



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:06 AM UTC

PDB ID : 3W68 / pdb_00003w68
Title : Crystal structure of mouse alpha-tocopherol transfer protein in complex with
alpha-tocopherol and phosphatidylinositol-(4,5)-bisphosphate
Authors : Ohto, U.; Satow, Y.
Deposited on : 2013-02-11
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

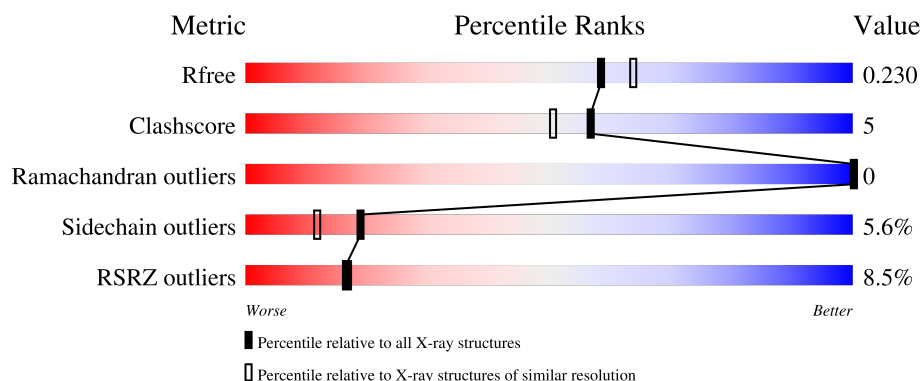
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	3% 83% 11% 6%
1	B	266	3% 79% 15% 5%
1	C	266	7% 79% 13% 5%
1	D	266	20% 78% 15% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-tocopherol transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2052	1324	357	364	7			
1	B	253	Total	C	N	O	S	0	0	0
			2068	1336	359	366	7			
1	C	252	Total	C	N	O	S	0	0	0
			2058	1329	357	365	7			
1	D	251	Total	C	N	O	S	0	0	0
			2052	1324	357	364	7			

There are 32 discrepancies between the modelled and reference sequences:

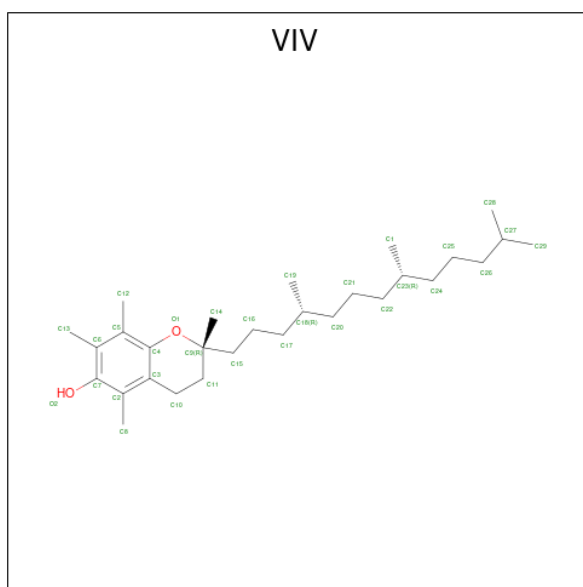
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q8BWP5
A	14	PRO	-	expression tag	UNP Q8BWP5
A	15	LEU	-	expression tag	UNP Q8BWP5
A	16	GLY	-	expression tag	UNP Q8BWP5
A	17	SER	-	expression tag	UNP Q8BWP5
A	18	PRO	-	expression tag	UNP Q8BWP5
A	19	GLU	-	expression tag	UNP Q8BWP5
A	20	PHE	-	expression tag	UNP Q8BWP5
B	13	GLY	-	expression tag	UNP Q8BWP5
B	14	PRO	-	expression tag	UNP Q8BWP5
B	15	LEU	-	expression tag	UNP Q8BWP5
B	16	GLY	-	expression tag	UNP Q8BWP5
B	17	SER	-	expression tag	UNP Q8BWP5
B	18	PRO	-	expression tag	UNP Q8BWP5
B	19	GLU	-	expression tag	UNP Q8BWP5
B	20	PHE	-	expression tag	UNP Q8BWP5
C	13	GLY	-	expression tag	UNP Q8BWP5
C	14	PRO	-	expression tag	UNP Q8BWP5
C	15	LEU	-	expression tag	UNP Q8BWP5
C	16	GLY	-	expression tag	UNP Q8BWP5
C	17	SER	-	expression tag	UNP Q8BWP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	PRO	-	expression tag	UNP Q8BWP5
C	19	GLU	-	expression tag	UNP Q8BWP5
C	20	PHE	-	expression tag	UNP Q8BWP5
D	13	GLY	-	expression tag	UNP Q8BWP5
D	14	PRO	-	expression tag	UNP Q8BWP5
D	15	LEU	-	expression tag	UNP Q8BWP5
D	16	GLY	-	expression tag	UNP Q8BWP5
D	17	SER	-	expression tag	UNP Q8BWP5
D	18	PRO	-	expression tag	UNP Q8BWP5
D	19	GLU	-	expression tag	UNP Q8BWP5
D	20	PHE	-	expression tag	UNP Q8BWP5

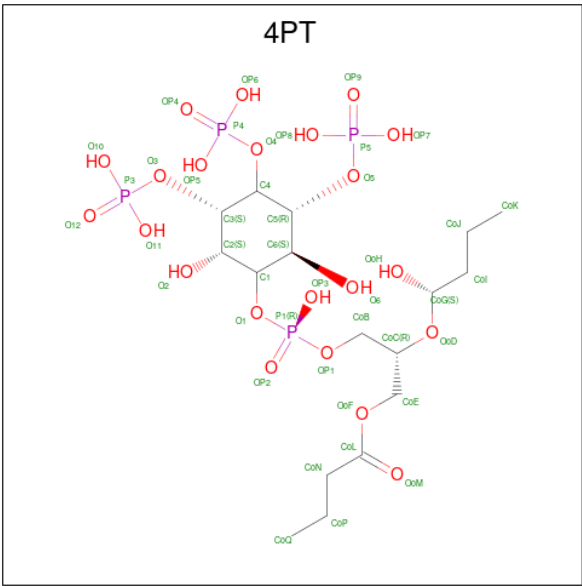
- Molecule 2 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (CCD ID: VIV) (formula: C₂₉H₅₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			31	29	2		
2	B	1	Total	C	O	0	0
			31	29	2		
2	C	1	Total	C	O	0	0
			31	29	2		
2	D	1	Total	C	O	0	0
			31	29	2		

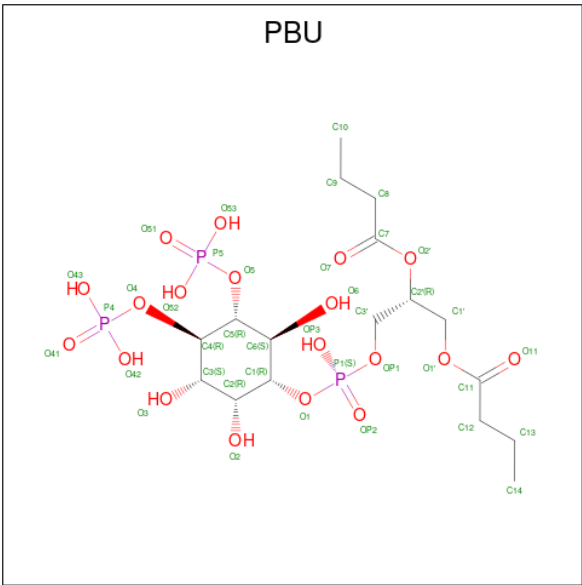
- Molecule 3 is (2R)-3-{[(S)-{[(2S,3R,5S,6S)-2,6-DIHYDROXY-3,4,5-TRIS(PHOSPHONOXY)CYCLOHEXYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-(1-HYDROXY

BUTOXY)PROPYL BUTYRATE (CCD ID: 4PT) (formula: C₁₇H₃₆O₂₂P₄).



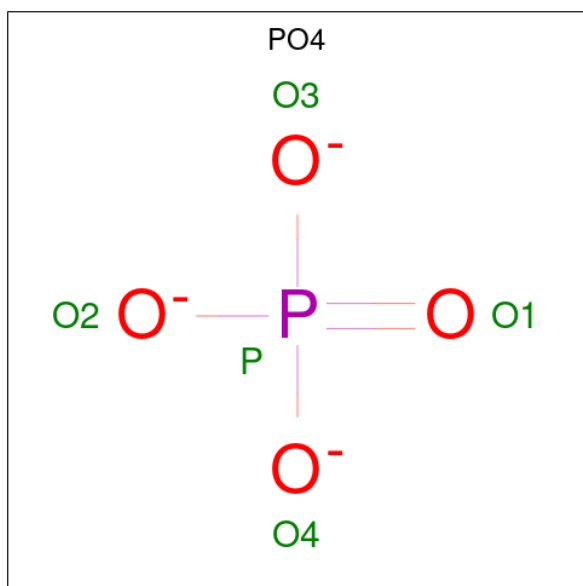
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			24	6	15	3		
3	A	1	Total	C	O	P	0	0
			24	6	15	3		
3	B	1	Total	C	O	P	0	0
			24	6	15	3		

- Molecule 4 is (2R)-3-{[(R)-HYDROXY{[(1R,2R,3S,4R,5R,6S)-2,3,6-TRIHYDROXY-4,5-BIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL]OXY}PROPANE-1,2-DIYL DIBUTANOATE (CCD ID: PBU) (formula: C₁₇H₃₃O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			39	17	19	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

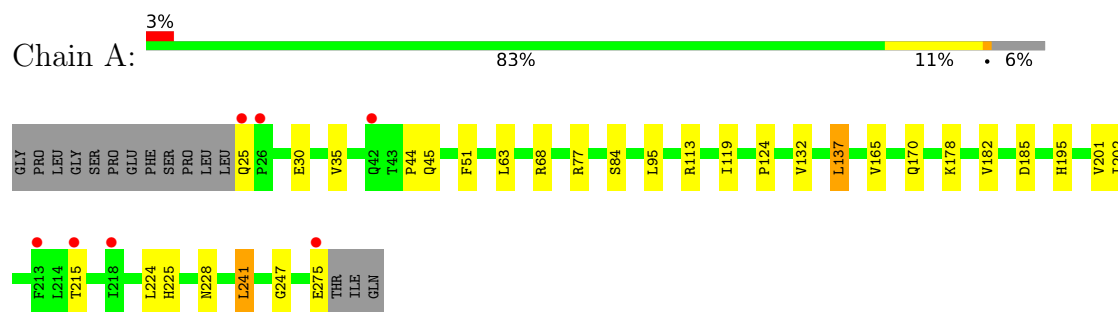
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total	O	0	0
			95	95		
6	B	86	Total	O	0	0
			86	86		
6	C	59	Total	O	0	0
			59	59		
6	D	7	Total	O	0	0
			7	7		

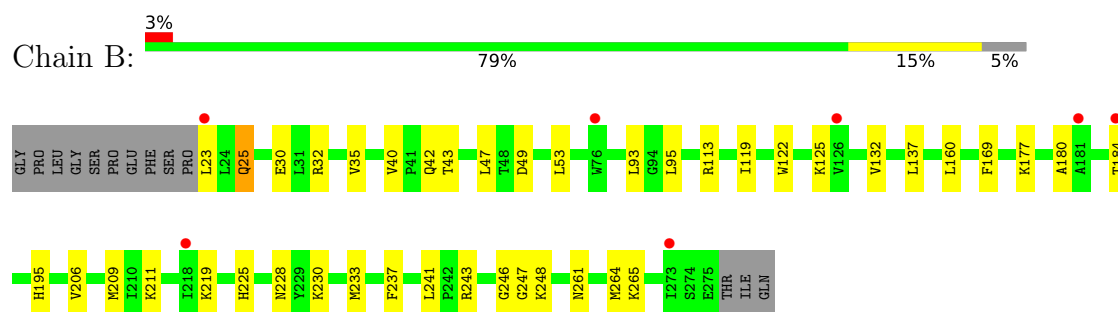
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

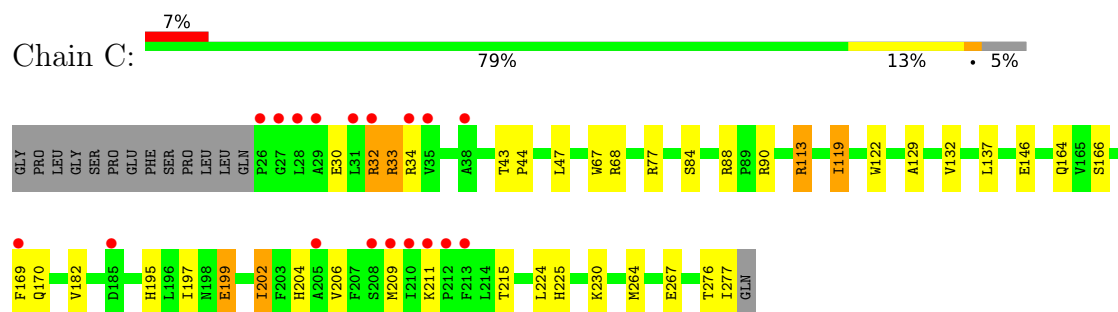
• Molecule 1: Alpha-tocopherol transfer protein



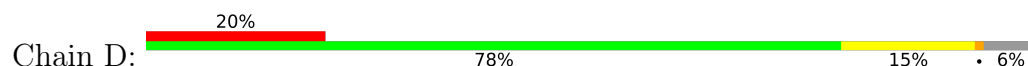
• Molecule 1: Alpha-tocopherol transfer protein

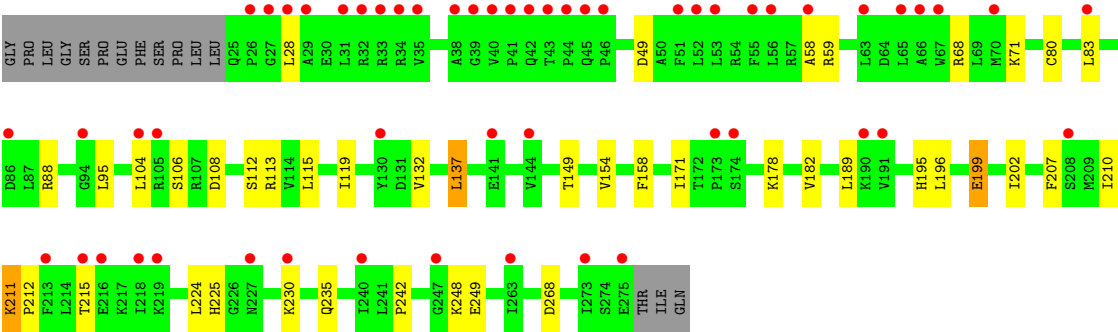


• Molecule 1: Alpha-tocopherol transfer protein



• Molecule 1: Alpha-tocopherol transfer protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.98Å 69.62Å 87.10Å 100.88° 109.45° 100.01°	Depositor
Resolution (Å)	29.32 – 2.05 29.32 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.32-2.05) 97.5 (29.32-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.231 0.199 , 0.230	Depositor DCC
R_{free} test set	3862 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8732	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PBU, PO4, 4PT, VIV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	0/2104	0.95	2/2848 (0.1%)
1	B	0.70	0/2120	0.93	2/2870 (0.1%)
1	C	0.66	0/2110	0.88	0/2856
1	D	0.53	0/2104	0.87	3/2848 (0.1%)
All	All	0.68	0/8438	0.91	7/11422 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	LEU	CA-C-N	-6.81	113.68	120.21
1	A	241	LEU	C-N-CA	-6.81	113.68	120.21
1	B	237	PHE	CA-C-N	-6.43	113.36	119.85
1	B	237	PHE	C-N-CA	-6.43	113.36	119.85
1	D	88	ARG	CA-C-N	5.74	125.28	119.19
1	D	88	ARG	C-N-CA	5.74	125.28	119.19
1	D	171	ILE	N-CA-C	5.18	111.75	106.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2052	0	2063	13	0
1	B	2068	0	2085	22	0
1	C	2058	0	2074	28	0
1	D	2052	0	2063	20	0
2	A	31	0	49	1	0
2	B	31	0	50	1	0
2	C	31	0	49	1	0
2	D	31	0	50	2	0
3	A	48	0	16	0	0
3	B	24	0	8	0	0
4	B	39	0	28	0	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
6	A	95	0	0	1	0
6	B	86	0	0	0	0
6	C	59	0	0	5	0
6	D	7	0	0	0	0
All	All	8732	0	8535	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:NH1	6:C:435:HOH:O	2.12	0.81
1:A:44:PRO:HG3	1:A:275:GLU:HG2	1.67	0.76
1:B:261:ASN:HB3	1:B:265:LYS:HZ1	1.53	0.74
1:B:169:PHE:HD2	1:C:169:PHE:CE1	2.06	0.74
1:B:195:HIS:ND1	1:B:225:HIS:HE1	1.88	0.71
1:B:261:ASN:HB3	1:B:265:LYS:NZ	2.07	0.69
1:A:195:HIS:ND1	1:A:225:HIS:HE1	1.93	0.67
1:B:32:ARG:NH1	1:B:49:ASP:OD1	2.28	0.66
1:C:195:HIS:ND1	1:C:225:HIS:HE1	1.96	0.64
1:C:32:ARG:NH2	1:C:47:LEU:O	2.30	0.63
1:B:230:LYS:HE2	1:B:246:GLY:HA2	1.83	0.61
1:C:264:MET:HE1	6:C:445:HOH:O	2.02	0.59
1:C:197:ILE:HG22	1:C:225:HIS:HB2	1.83	0.59
1:A:95:LEU:HD21	1:A:132:VAL:HG22	1.83	0.59
1:C:267:GLU:OE1	6:C:445:HOH:O	2.18	0.56
1:C:119:ILE:HD13	1:C:122:TRP:HE3	1.70	0.56
1:D:58:ALA:O	1:D:59:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:NH1	1:C:146:GLU:OE2	2.40	0.55
1:B:95:LEU:HD21	1:B:132:VAL:HG22	1.88	0.54
1:C:88:ARG:NH2	6:C:426:HOH:O	2.40	0.54
1:B:169:PHE:CD2	1:C:169:PHE:CE1	2.92	0.53
1:D:83:LEU:HD12	1:D:178:LYS:HE2	1.90	0.53
1:A:201:VAL:HG11	1:C:204:HIS:HB3	1.91	0.53
1:C:68:ARG:HD2	1:D:68:ARG:HH11	1.74	0.52
1:B:35:VAL:HG13	1:B:40:VAL:HB	1.90	0.52
1:D:113:ARG:HB2	1:D:154:VAL:HG12	1.92	0.52
1:B:241:LEU:O	1:B:247:GLY:HA3	2.10	0.51
1:C:202:ILE:O	1:C:206:VAL:HG22	2.12	0.49
1:C:122:TRP:CE2	1:C:132:VAL:HG21	2.47	0.48
1:A:45:GLN:HG2	1:A:51:PHE:CE1	2.49	0.48
1:B:180:ALA:O	1:B:184:THR:HG23	2.13	0.48
1:D:95:LEU:HD21	1:D:132:VAL:HG22	1.96	0.48
1:D:68:ARG:HA	1:D:71:LYS:HE3	1.96	0.48
1:B:169:PHE:HD2	1:C:169:PHE:HE1	1.59	0.48
1:B:206:VAL:HA	1:B:209:MET:HE3	1.95	0.48
1:D:248:LYS:HG3	1:D:249:GLU:HG3	1.95	0.48
1:A:68:ARG:NH1	1:A:185:ASP:OD1	2.47	0.47
1:C:199:GLU:H	1:C:199:GLU:CD	2.23	0.47
1:D:80:CYS:SG	1:D:178:LYS:HE3	2.54	0.47
1:B:25:GLN:HG2	1:B:53:LEU:HD21	1.97	0.47
1:D:158:PHE:HB2	1:D:196:LEU:HD23	1.97	0.46
1:A:30:GLU:CG	1:A:63:LEU:HD21	2.45	0.46
1:C:129:ALA:HB2	1:C:170:GLN:HB3	1.98	0.46
1:D:211:LYS:HB3	1:D:212:PRO:HD3	1.97	0.46
1:C:164:GLN:NE2	1:C:166:SER:OG	2.49	0.46
1:A:137:LEU:HD13	2:A:301:VIV:C12	2.46	0.46
1:D:104:LEU:HD21	1:D:242:PRO:HD3	1.98	0.45
1:D:108:ASP:OD1	1:D:112:SER:HB2	2.16	0.45
1:D:149:THR:HG22	1:D:189:LEU:HD21	1.98	0.45
1:B:169:PHE:CD2	1:C:169:PHE:HE1	2.32	0.45
1:D:137:LEU:HD13	2:D:301:VIV:C12	2.47	0.45
2:D:301:VIV:H191	2:D:301:VIV:H211	1.86	0.45
1:A:124:PRO:O	1:A:170:GLN:NE2	2.51	0.44
1:B:32:ARG:NH2	1:B:47:LEU:O	2.50	0.44
1:B:119:ILE:HG13	1:B:160:LEU:HD23	1.98	0.44
1:A:241:LEU:O	1:A:247:GLY:HA3	2.17	0.44
1:B:230:LYS:HE2	1:B:246:GLY:CA	2.47	0.44
1:C:68:ARG:HD2	1:D:68:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HG2	1:A:84:SER:HB2	2.00	0.44
1:B:243:ARG:HG2	1:B:248:LYS:HA	1.99	0.44
1:B:211:LYS:O	1:B:219:LYS:HE2	2.18	0.43
1:D:195:HIS:ND1	1:D:225:HIS:HE1	2.15	0.43
1:C:113:ARG:HH11	1:C:146:GLU:CD	2.26	0.43
2:B:301:VIV:H191	2:B:301:VIV:H211	1.78	0.43
1:C:34:ARG:HH11	1:C:67:TRP:CD1	2.37	0.43
1:C:33:ARG:HB3	1:C:33:ARG:CZ	2.49	0.43
2:C:301:VIV:H191	2:C:301:VIV:H211	1.90	0.43
1:D:199:GLU:H	1:D:199:GLU:CD	2.27	0.42
1:D:196:LEU:HD12	1:D:224:LEU:HG	2.01	0.42
1:A:178:LYS:HE3	6:A:481:HOH:O	2.19	0.42
1:D:28:LEU:HD11	1:D:49:ASP:HB3	2.00	0.42
1:C:90:ARG:HB2	6:C:445:HOH:O	2.20	0.42
1:C:43:THR:HB	1:C:44:PRO:HA	2.02	0.41
1:B:93:LEU:HD13	1:B:264:MET:SD	2.61	0.41
1:C:122:TRP:CD2	1:C:132:VAL:HG21	2.55	0.41
1:D:207:PHE:HA	1:D:210:ILE:HG22	2.01	0.40
1:C:77:ARG:HG2	1:C:84:SER:HB2	2.03	0.40
1:B:122:TRP:CD2	1:B:132:VAL:HG21	2.56	0.40
1:A:30:GLU:HG2	1:A:63:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/266 (94%)	244 (98%)	5 (2%)	0	100	100
1	B	251/266 (94%)	247 (98%)	4 (2%)	0	100	100
1	C	250/266 (94%)	244 (98%)	6 (2%)	0	100	100
1	D	249/266 (94%)	241 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	999/1064 (94%)	976 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/236 (94%)	212 (95%)	11 (5%)	22	15
1	B	225/236 (95%)	214 (95%)	11 (5%)	22	15
1	C	224/236 (95%)	208 (93%)	16 (7%)	13	7
1	D	223/236 (94%)	211 (95%)	12 (5%)	20	12
All	All	895/944 (95%)	845 (94%)	50 (6%)	19	12

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	35	VAL
1	A	113	ARG
1	A	119	ILE
1	A	137	LEU
1	A	165	VAL
1	A	182	VAL
1	A	202	ILE
1	A	215	THR
1	A	224	LEU
1	A	228	ASN
1	B	23	LEU
1	B	25	GLN
1	B	30	GLU
1	B	42	GLN
1	B	43	THR
1	B	113	ARG

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Mol	Chain	Res	Type
1	B	125	LYS
1	B	137	LEU
1	B	177	LYS
1	B	228	ASN
1	B	233	MET
1	C	30	GLU
1	C	32	ARG
1	C	33	ARG
1	C	113	ARG
1	C	119	ILE
1	C	137	LEU
1	C	182	VAL
1	C	199	GLU
1	C	202	ILE
1	C	209	MET
1	C	211	LYS
1	C	215	THR
1	C	224	LEU
1	C	230	LYS
1	C	276	THR
1	C	277	ILE
1	D	106	SER
1	D	115	LEU
1	D	119	ILE
1	D	137	LEU
1	D	182	VAL
1	D	199	GLU
1	D	202	ILE
1	D	211	LYS
1	D	215	THR
1	D	230	LYS
1	D	235	GLN
1	D	268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	42	GLN
1	A	45	GLN
1	A	152	ASN
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	225	HIS
1	B	25	GLN
1	B	42	GLN
1	B	145	GLN
1	B	152	ASN
1	B	225	HIS
1	B	257	GLN
1	C	145	GLN
1	C	164	GLN
1	C	225	HIS
1	C	227	ASN
1	C	236	HIS
1	C	257	GLN
1	D	145	GLN
1	D	152	ASN
1	D	164	GLN
1	D	225	HIS
1	D	235	GLN
1	D	236	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VIV	D	301	-	32,32,32	0.99	2 (6%)	43,45,45	1.19	6 (13%)
5	PO4	D	302	-	4,4,4	0.92	0	6,6,6	0.56	0
5	PO4	C	303	-	4,4,4	0.86	0	6,6,6	0.66	0
2	VIV	A	301	-	32,32,32	1.04	2 (6%)	43,45,45	1.29	5 (11%)
5	PO4	C	304	-	4,4,4	0.95	0	6,6,6	0.53	0
2	VIV	B	301	-	32,32,32	1.21	5 (15%)	43,45,45	1.08	3 (6%)
2	VIV	C	301	-	32,32,32	1.12	3 (9%)	43,45,45	1.16	5 (11%)
5	PO4	C	302	-	4,4,4	0.93	0	6,6,6	0.57	0
3	4PT	A	302	-	24,24,43	1.99	7 (29%)	39,39,64	1.07	1 (2%)
4	PBU	B	302	-	39,39,39	1.85	8 (20%)	54,57,57	1.54	7 (12%)
3	4PT	B	303	-	24,24,43	1.73	7 (29%)	39,39,64	0.83	0
3	4PT	A	303	-	24,24,43	1.60	7 (29%)	39,39,64	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VIV	D	301	-	-	4/19/30/30	0/2/2/2
2	VIV	A	301	-	-	4/19/30/30	0/2/2/2
2	VIV	B	301	-	-	5/19/30/30	0/2/2/2
2	VIV	C	301	-	-	5/19/30/30	0/2/2/2
3	4PT	A	302	-	-	3/15/39/65	0/1/1/1
4	PBU	B	302	-	-	4/36/60/60	0/1/1/1
3	4PT	B	303	-	-	2/15/39/65	0/1/1/1
3	4PT	A	303	-	-	1/15/39/65	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	PBU	O7-C7	6.98	1.43	1.22
3	A	302	4PT	P4-OP4	4.25	1.63	1.50
3	A	302	4PT	P1-OP2	4.25	1.63	1.50
3	A	303	4PT	P1-OP2	4.08	1.63	1.50
3	B	303	4PT	P1-OP2	4.04	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	PBU	P1-OP2	3.76	1.63	1.50
4	B	302	PBU	P5-O51	3.74	1.62	1.50
3	A	302	4PT	P5-OP9	3.71	1.62	1.50
3	B	303	4PT	P5-O5	3.35	1.65	1.59
4	B	302	PBU	P4-O41	3.30	1.60	1.50
2	C	301	VIV	C21-C20	-3.02	1.39	1.52
2	C	301	VIV	C21-C22	-2.90	1.40	1.52
4	B	302	PBU	P5-O52	2.87	1.65	1.54
4	B	302	PBU	O2'-C7	2.87	1.42	1.34
2	B	301	VIV	C21-C22	-2.84	1.40	1.52
2	B	301	VIV	C21-C20	-2.74	1.40	1.52
3	A	302	4PT	P4-O4	2.67	1.64	1.59
2	D	301	VIV	C21-C20	-2.67	1.41	1.52
3	B	303	4PT	P4-OP6	2.66	1.64	1.54
3	A	302	4PT	P5-O5	2.65	1.64	1.59
2	A	301	VIV	C21-C22	-2.64	1.41	1.52
2	A	301	VIV	C21-C20	-2.62	1.41	1.52
3	B	303	4PT	P1-O1	2.59	1.64	1.59
2	D	301	VIV	C21-C22	-2.58	1.41	1.52
3	B	303	4PT	P1-OP3	2.54	1.64	1.54
3	A	302	4PT	P5-OP7	2.48	1.64	1.54
3	A	302	4PT	P1-OP3	2.44	1.63	1.54
3	A	303	4PT	P5-O5	2.34	1.63	1.59
2	B	301	VIV	C10-C3	2.32	1.55	1.51
2	B	301	VIV	C8-C2	2.28	1.56	1.51
3	A	303	4PT	P1-OP1	2.22	1.63	1.54
3	B	303	4PT	P5-OP7	2.17	1.62	1.54
3	A	303	4PT	P1-O1	2.13	1.63	1.59
2	C	301	VIV	C14-C9	2.13	1.56	1.52
3	B	303	4PT	P4-OP5	2.10	1.62	1.54
3	A	303	4PT	P5-OP7	2.06	1.62	1.54
3	A	303	4PT	P4-OP6	2.05	1.62	1.54
3	A	303	4PT	P5-OP8	2.03	1.62	1.54
4	B	302	PBU	C8-C7	2.01	1.56	1.50
4	B	302	PBU	P4-O43	-2.01	1.47	1.54
2	B	301	VIV	O1-C9	-2.01	1.44	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	PBU	O2'-C7-O7	-7.22	106.84	123.70
2	A	301	VIV	C10-C11-C9	-4.46	108.06	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	VIV	C10-C11-C9	3.17	113.70	111.36
2	B	301	VIV	O1-C9-C11	3.04	110.58	108.78
2	D	301	VIV	C21-C22-C23	2.93	125.69	115.97
4	B	302	PBU	O7-C7-C8	-2.83	112.73	123.78
2	D	301	VIV	C22-C21-C20	2.80	125.82	113.28
2	C	301	VIV	C21-C22-C23	2.71	124.96	115.97
4	B	302	PBU	C2'-O2'-C7	-2.68	111.38	117.80
2	C	301	VIV	O1-C9-C14	2.65	111.91	105.47
2	A	301	VIV	C22-C21-C20	2.62	125.00	113.28
2	A	301	VIV	C21-C22-C23	2.58	124.53	115.97
2	C	301	VIV	C22-C21-C20	2.47	124.34	113.28
3	A	302	4PT	P5-O5-C5	-2.42	116.98	123.43
2	D	301	VIV	C7-C2-C3	2.34	121.42	118.59
2	B	301	VIV	C22-C21-C20	2.33	123.73	113.28
2	B	301	VIV	C21-C22-C23	2.29	123.59	115.97
4	B	302	PBU	O52-P5-O51	-2.28	101.96	110.83
4	B	302	PBU	O2'-C2'-C1'	2.26	116.44	108.34
4	B	302	PBU	O43-P4-O41	2.22	119.50	110.83
2	A	301	VIV	O1-C9-C14	2.19	110.80	105.47
2	C	301	VIV	O1-C4-C3	-2.13	120.20	122.36
4	B	302	PBU	O53-P5-O5	2.09	113.99	105.85
2	D	301	VIV	C4-C5-C6	2.06	120.72	118.77
2	A	301	VIV	C15-C16-C17	-2.03	108.78	112.68
2	D	301	VIV	O1-C4-C5	2.03	117.57	115.41
2	C	301	VIV	C10-C11-C9	2.00	112.84	111.36

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	VIV	C20-C21-C22-C23
2	B	301	VIV	C20-C21-C22-C23
2	C	301	VIV	C20-C21-C22-C23
2	D	301	VIV	C20-C21-C22-C23
2	B	301	VIV	C23-C24-C25-C26
4	B	302	PBU	O7-C7-O2'-C2'
4	B	302	PBU	O1'-C1'-C2'-C3'
2	B	301	VIV	C18-C20-C21-C22
2	D	301	VIV	C18-C20-C21-C22
2	C	301	VIV	C18-C20-C21-C22
4	B	302	PBU	O1'-C1'-C2'-O2'
2	C	301	VIV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	301	VIV	C21-C22-C23-C1
2	C	301	VIV	C21-C22-C23-C24
2	A	301	VIV	C18-C20-C21-C22
2	B	301	VIV	C21-C22-C23-C1
2	B	301	VIV	C21-C22-C23-C24
3	A	303	4PT	C5-O5-P5-OP8
4	B	302	PBU	C4-O4-P4-O43
3	A	302	4PT	C4-O4-P4-OP4
2	A	301	VIV	C21-C22-C23-C1
2	D	301	VIV	C21-C22-C23-C1
2	A	301	VIV	C21-C22-C23-C24
2	D	301	VIV	C23-C24-C25-C26
3	B	303	4PT	C2-C1-O1-P1
3	B	303	4PT	C3-C4-O4-P4
3	A	302	4PT	C4-O4-P4-OP5
3	A	302	4PT	C5-O5-P5-OP8

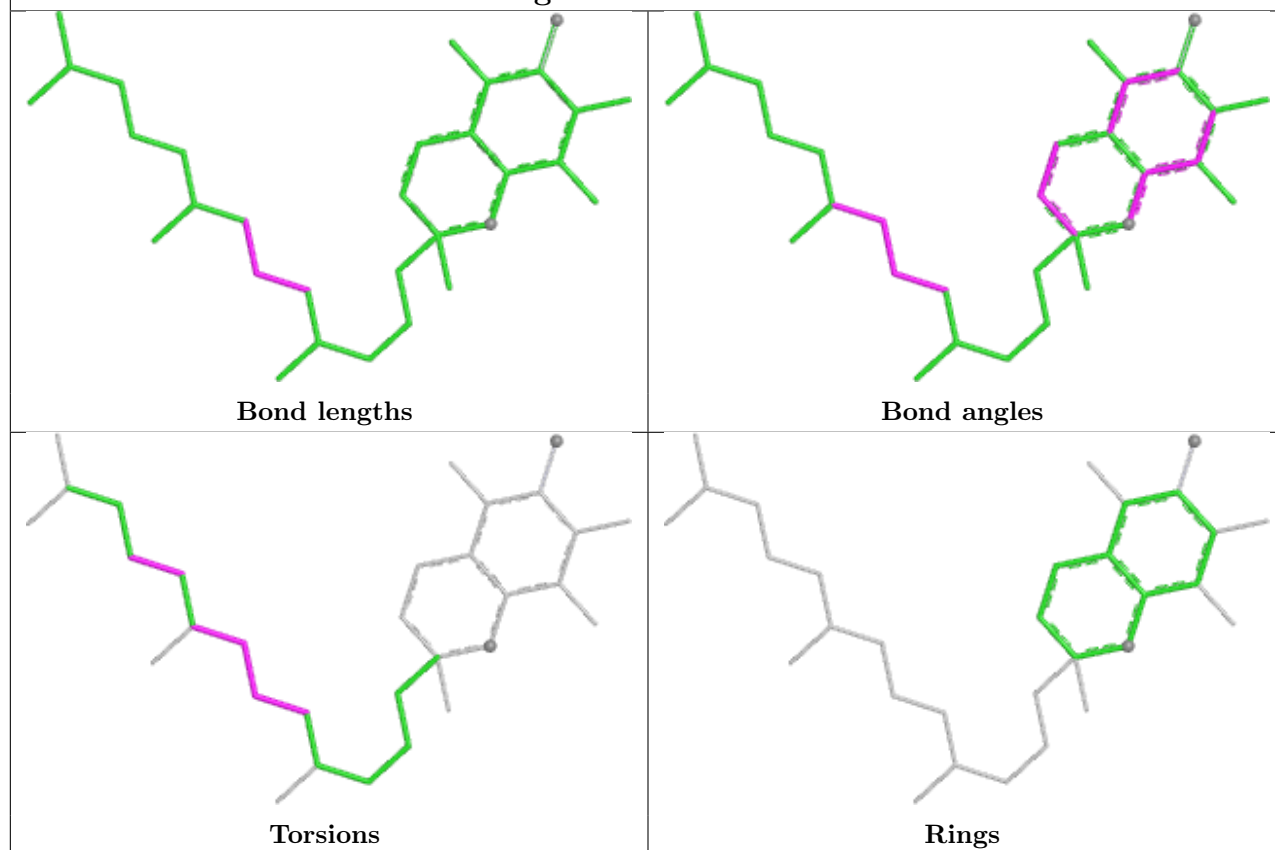
There are no ring outliers.

4 monomers are involved in 5 short contacts:

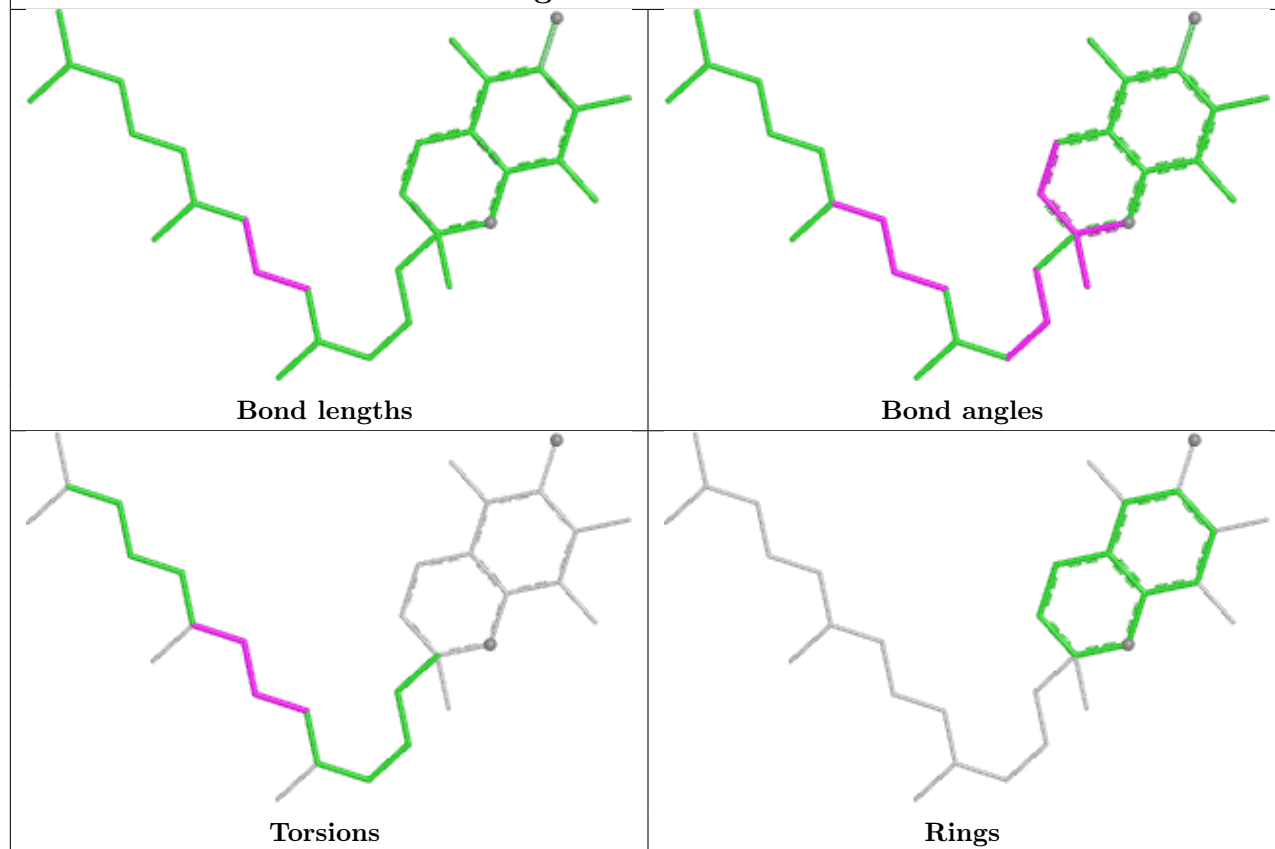
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	VIV	2	0
2	A	301	VIV	1	0
2	B	301	VIV	1	0
2	C	301	VIV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

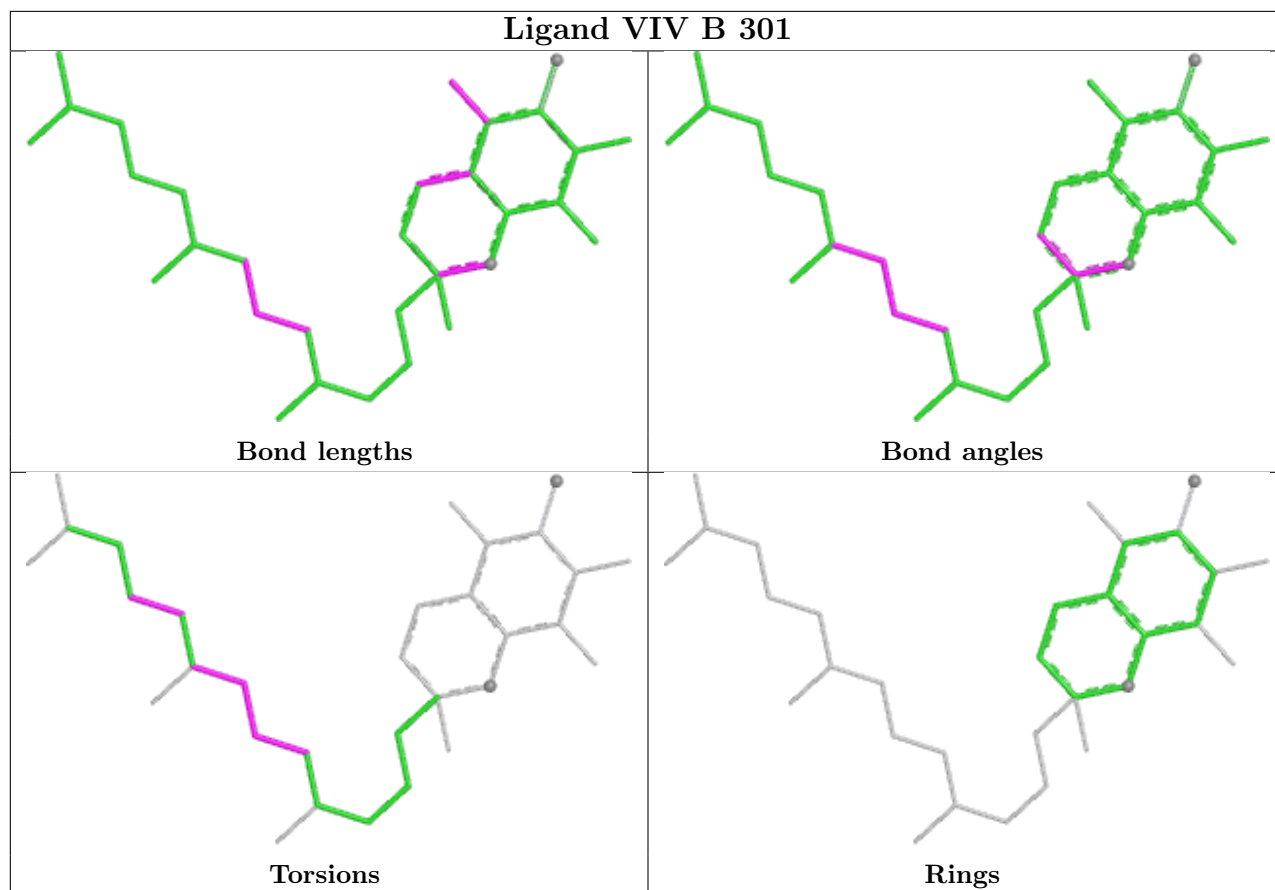
Ligand VIV D 301



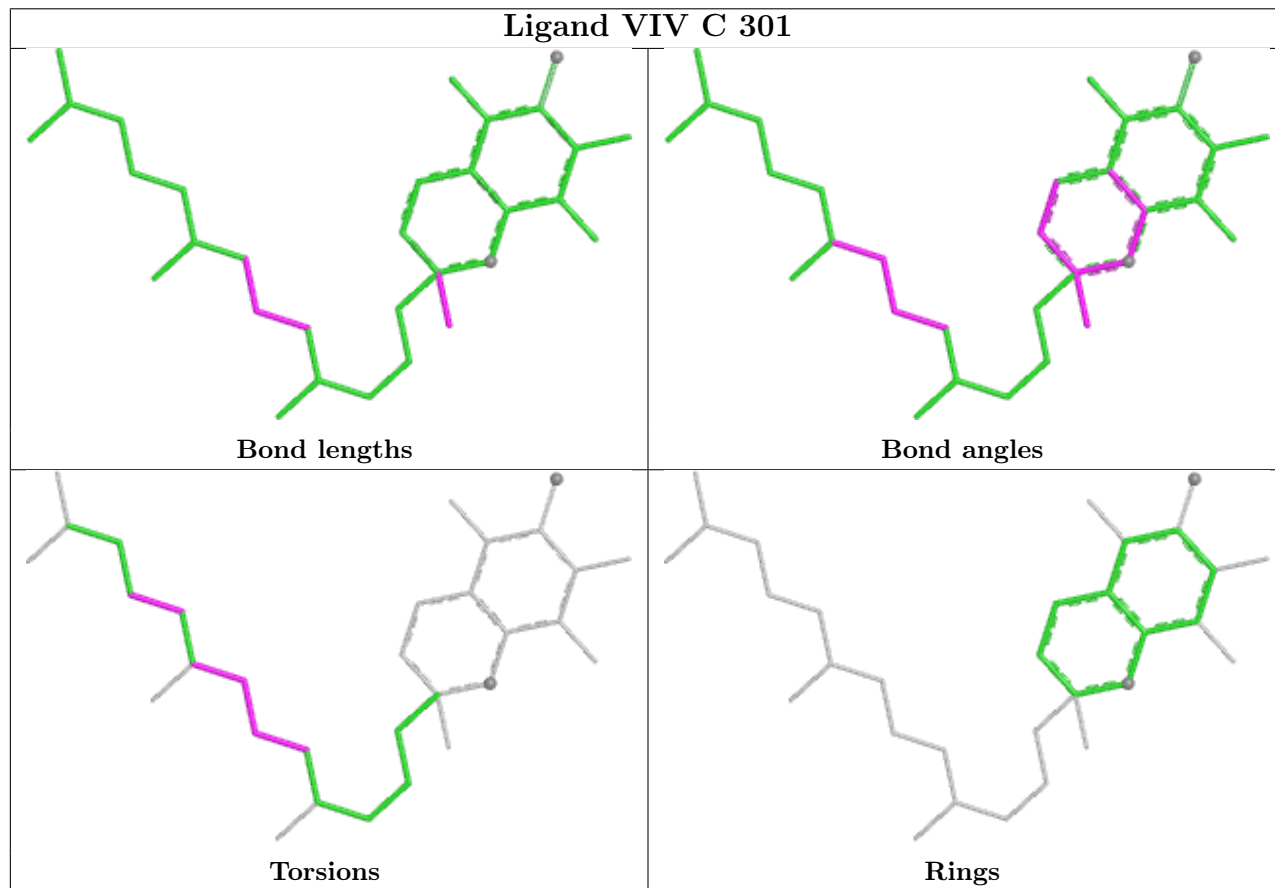
Ligand VIV A 301



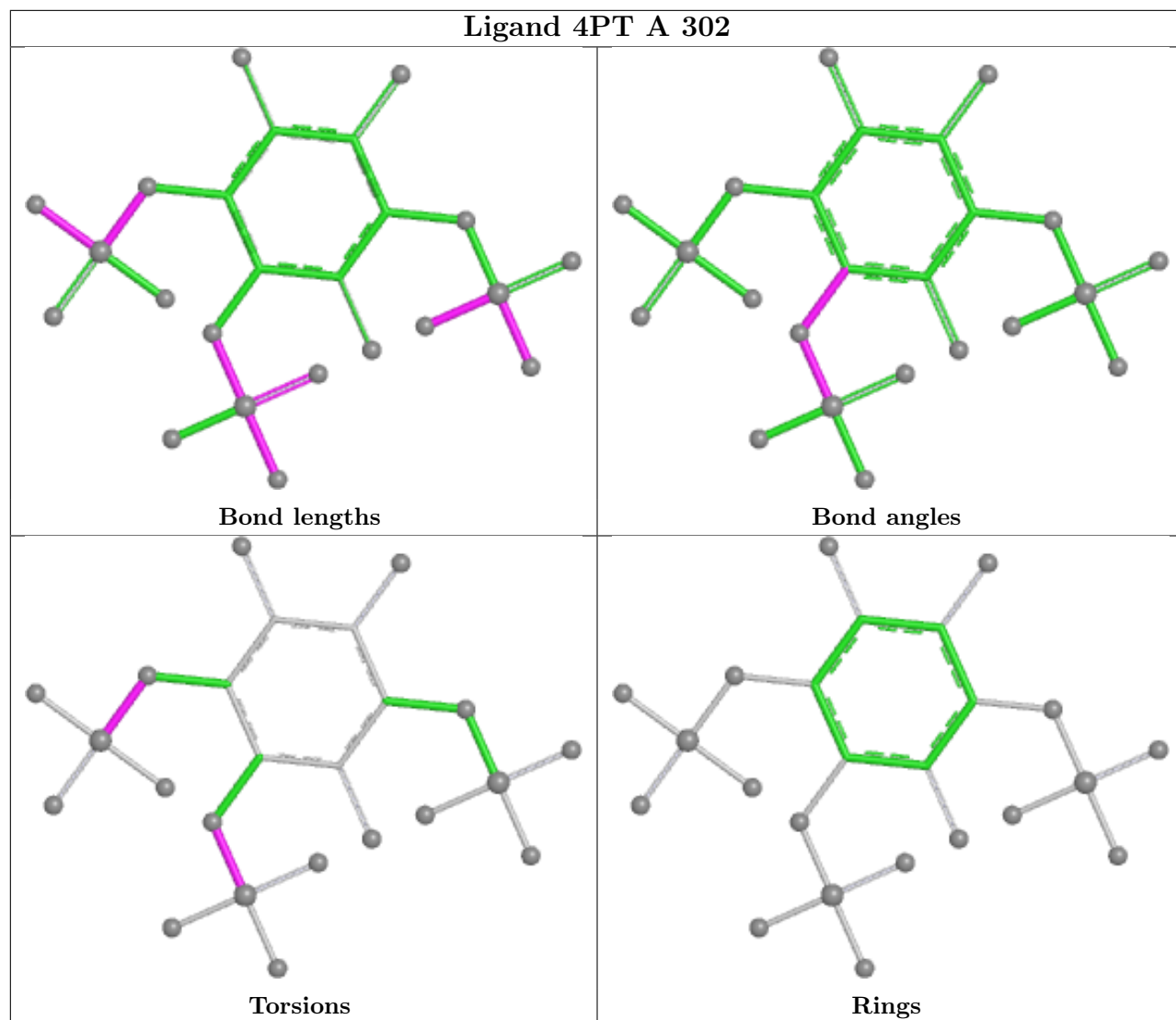
Ligand VIV B 301

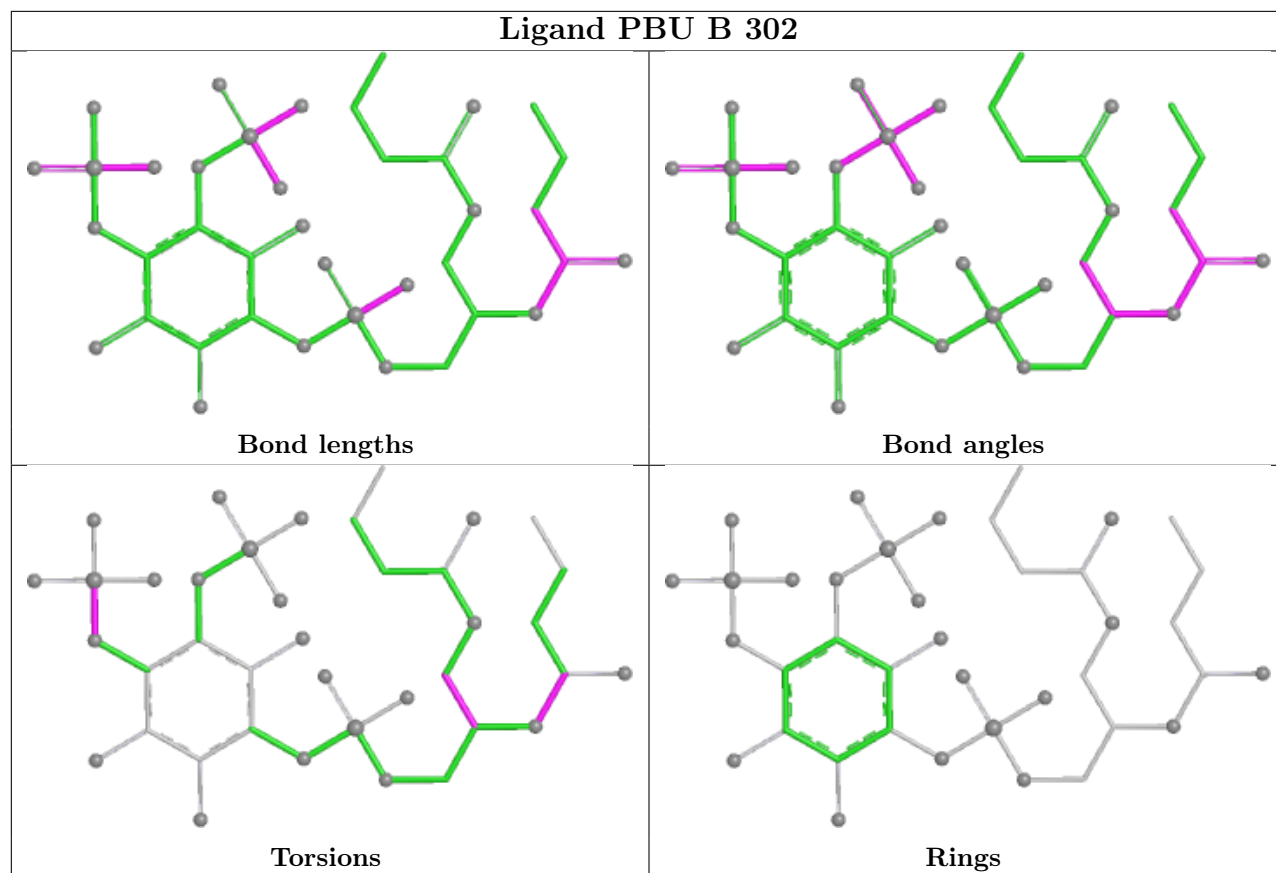


Ligand VIV C 301

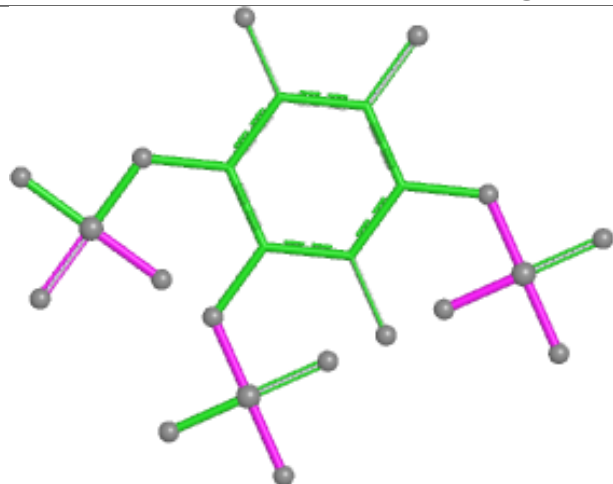


Ligand 4PT A 302

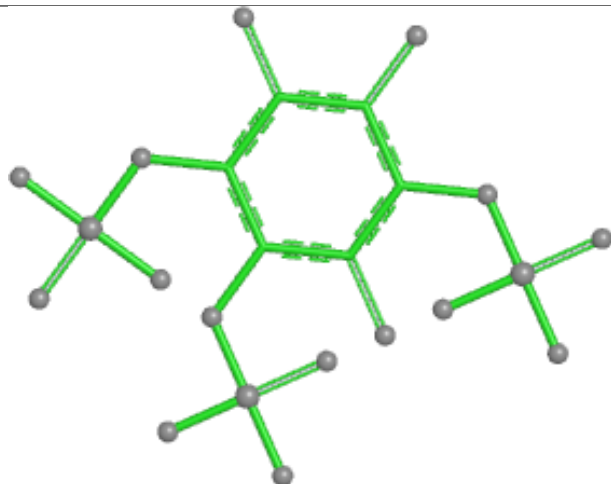




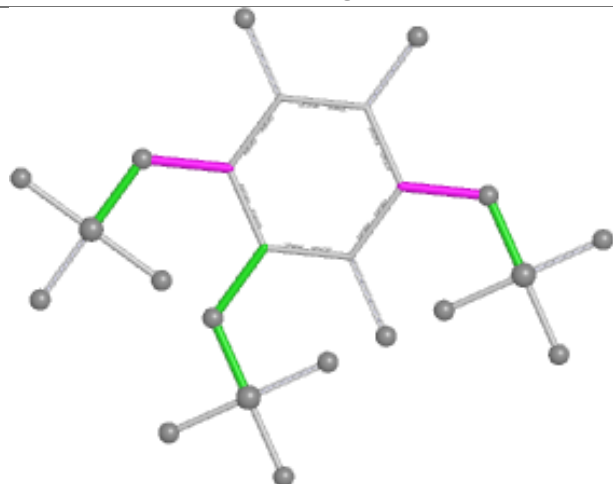
Ligand 4PT B 303



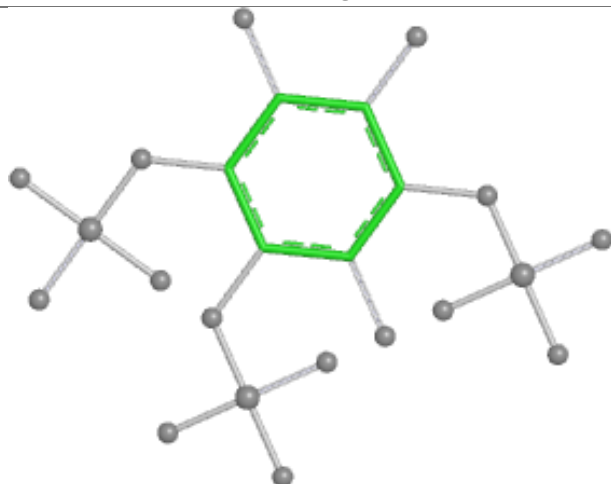
Bond lengths



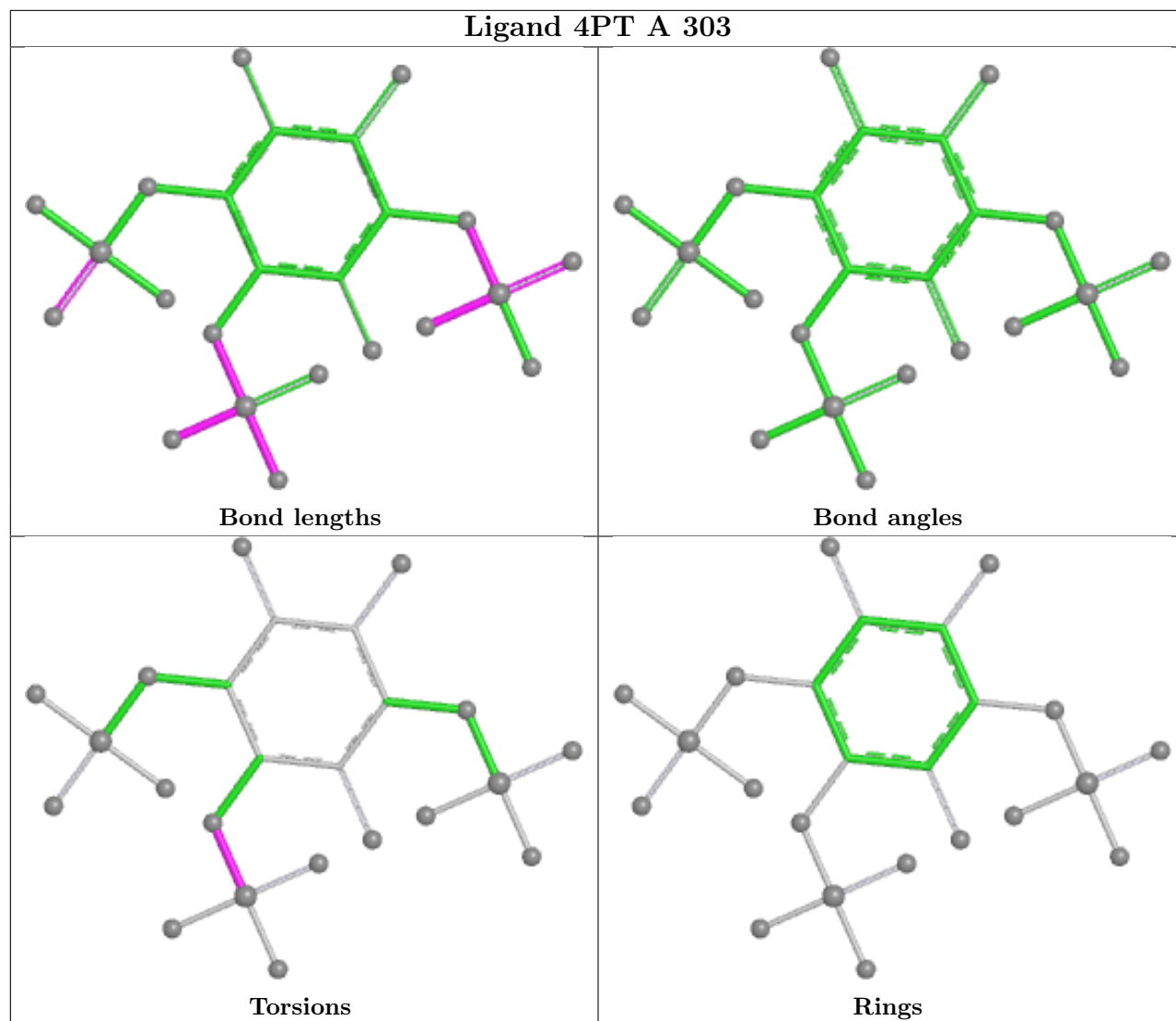
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/266 (94%)	0.28	7 (2%) 55 57	37, 55, 89, 103	0
1	B	253/266 (95%)	0.40	7 (2%) 55 57	40, 63, 92, 109	0
1	C	252/266 (94%)	0.62	18 (7%) 22 22	45, 64, 101, 219	0
1	D	251/266 (94%)	1.35	54 (21%) 2 1	65, 98, 213, 264	0
All	All	1007/1064 (94%)	0.66	86 (8%) 16 17	37, 67, 128, 264	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	8.0
1	C	31	LEU	5.7
1	C	35	VAL	5.3
1	D	28	LEU	4.9
1	D	44	PRO	4.9
1	C	38	ALA	4.8
1	D	27	GLY	4.8
1	C	26	PRO	4.8
1	D	31	LEU	4.6
1	D	43	THR	4.4
1	D	141	GLU	4.4
1	D	45	GLN	4.3
1	D	56	LEU	4.2
1	C	32	ARG	3.9
1	C	27	GLY	3.8
1	C	29	ALA	3.7
1	D	26	PRO	3.6
1	D	58	ALA	3.4
1	D	35	VAL	3.4
1	D	40	VAL	3.3
1	D	191	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	208	SER	3.2
1	D	219	LYS	3.2
1	D	41	PRO	3.2
1	D	52	LEU	3.2
1	D	240	ILE	3.2
1	C	205	ALA	3.1
1	A	215	THR	3.1
1	D	34	ARG	3.1
1	D	38	ALA	2.9
1	C	213	PHE	2.9
1	D	53	LEU	2.8
1	B	23	LEU	2.8
1	D	39	GLY	2.8
1	A	218	ILE	2.8
1	D	213	PHE	2.7
1	D	63	LEU	2.7
1	D	208	SER	2.7
1	D	66	ALA	2.6
1	D	32	ARG	2.6
1	D	190	LYS	2.6
1	D	227	ASN	2.5
1	D	33	ARG	2.5
1	C	212	PRO	2.5
1	A	42	GLN	2.5
1	D	173	PRO	2.5
1	D	65	LEU	2.5
1	D	83	LEU	2.5
1	B	184	THR	2.4
1	D	46	PRO	2.4
1	D	42	GLN	2.4
1	D	67	TRP	2.4
1	D	230	LYS	2.3
1	D	29	ALA	2.3
1	D	70	MET	2.3
1	C	210	ILE	2.3
1	A	275	GLU	2.3
1	D	215	THR	2.3
1	C	34	ARG	2.3
1	C	209	MET	2.3
1	D	216	GLU	2.3
1	D	144	VAL	2.3
1	D	105	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	2.3
1	D	51	PHE	2.2
1	B	218	ILE	2.2
1	C	169	PHE	2.2
1	C	185	ASP	2.2
1	D	275	GLU	2.2
1	B	76	TRP	2.2
1	A	26	PRO	2.2
1	D	273	ILE	2.1
1	D	174	SER	2.1
1	C	211	LYS	2.1
1	D	130	TYR	2.1
1	D	94	GLY	2.1
1	A	213	PHE	2.1
1	D	55	PHE	2.1
1	A	25	GLN	2.1
1	B	273	ILE	2.1
1	D	263	ILE	2.1
1	D	86	ASP	2.0
1	D	247	GLY	2.0
1	D	218	ILE	2.0
1	B	126	VAL	2.0
1	D	104	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Continued on next page...

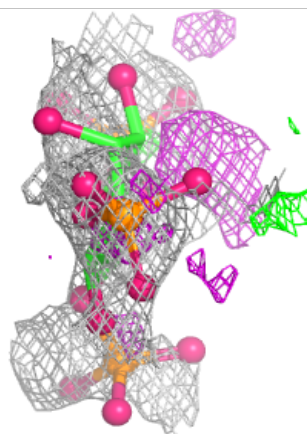
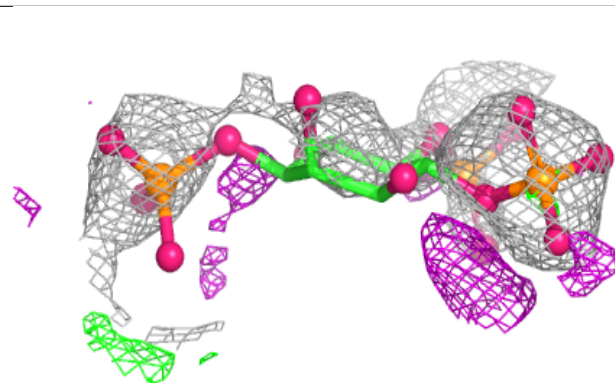
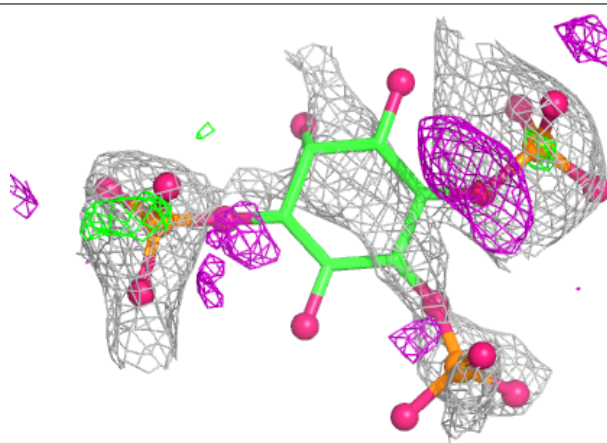
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	D	302	5/5	0.59	0.12	149,149,149,149	0
3	4PT	A	303	24/43	0.61	0.15	151,157,158,159	0
5	PO4	C	304	5/5	0.63	0.08	143,143,143,143	0
5	PO4	C	302	5/5	0.63	0.12	117,117,117,117	0
3	4PT	B	303	24/43	0.76	0.13	89,106,112,113	0
3	4PT	A	302	24/43	0.79	0.10	87,96,98,99	0
5	PO4	C	303	5/5	0.84	0.11	98,98,99,100	0
2	VIV	D	301	31/31	0.90	0.13	68,73,77,78	0
4	PBU	B	302	39/39	0.92	0.11	58,66,73,76	0
2	VIV	C	301	31/31	0.94	0.10	46,54,63,65	0
2	VIV	B	301	31/31	0.94	0.09	53,56,60,62	0
2	VIV	A	301	31/31	0.95	0.09	39,45,56,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

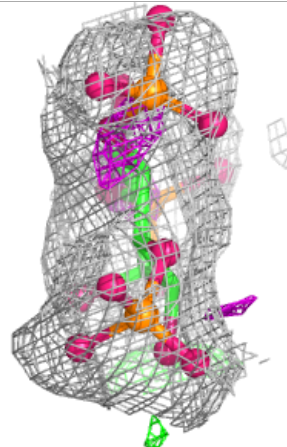
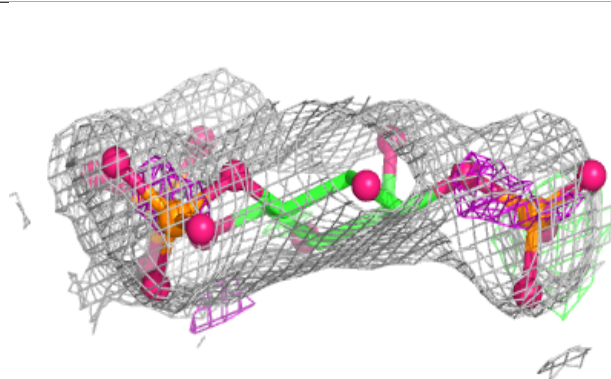
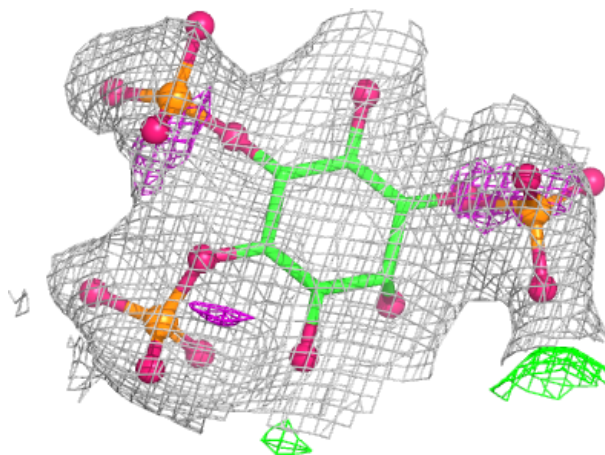
Electron density around 4PT A 303:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



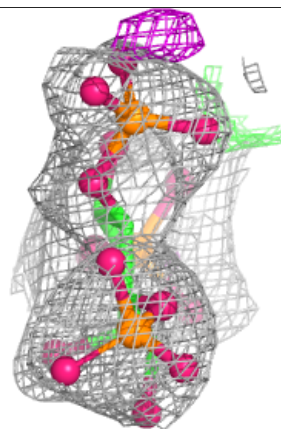
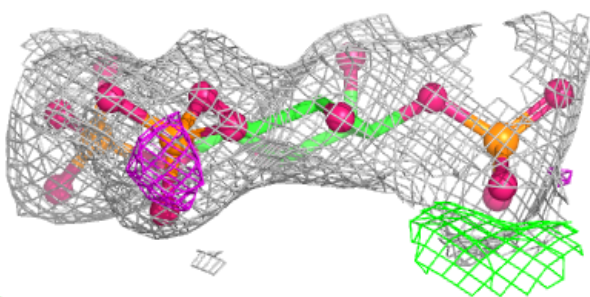
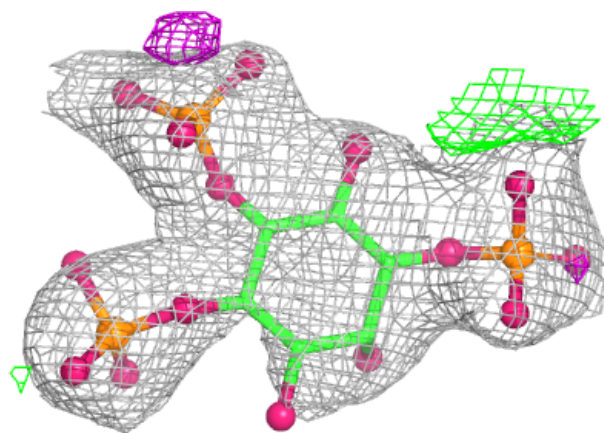
Electron density around 4PT B 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

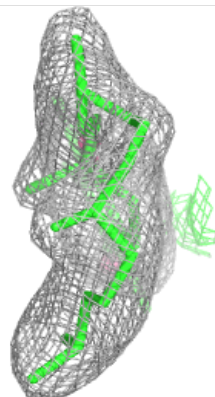
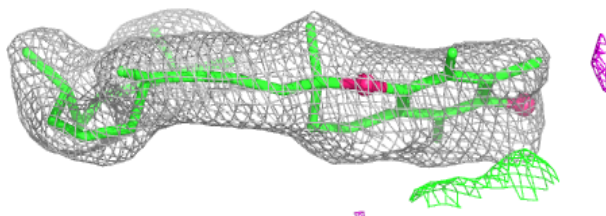
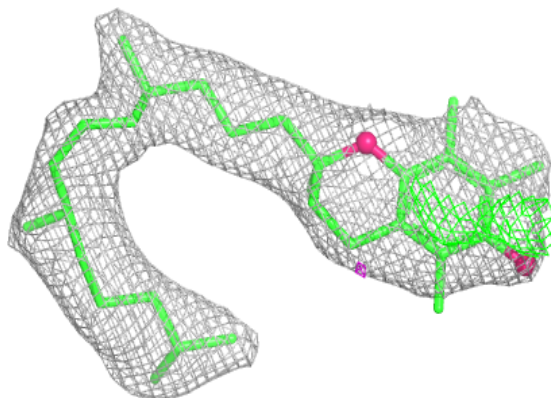


Electron density around 4PT A 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

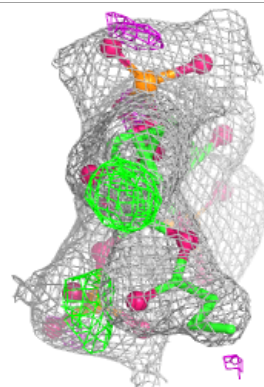
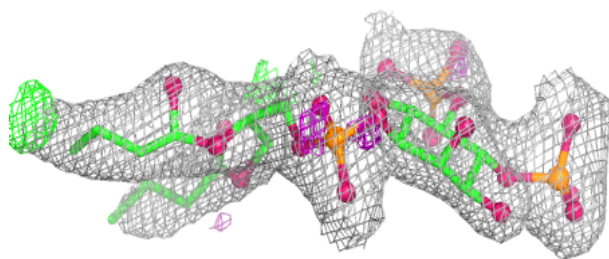
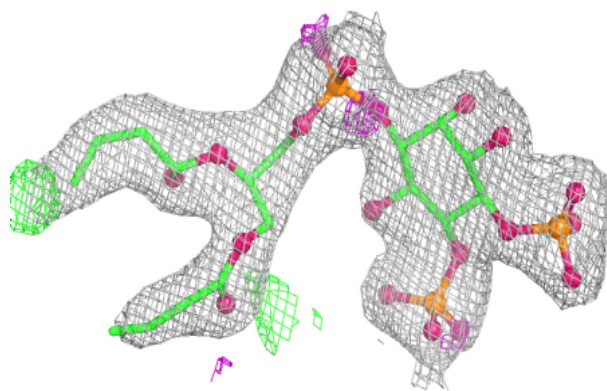
**Electron density around VIV D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

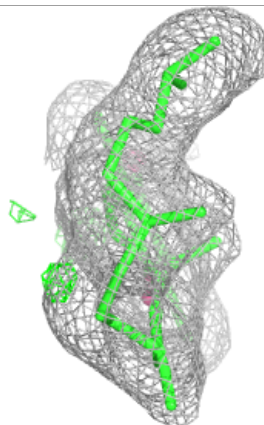
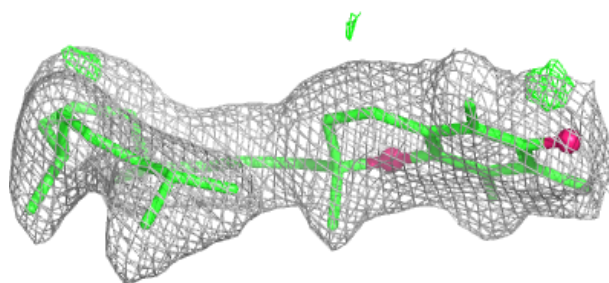
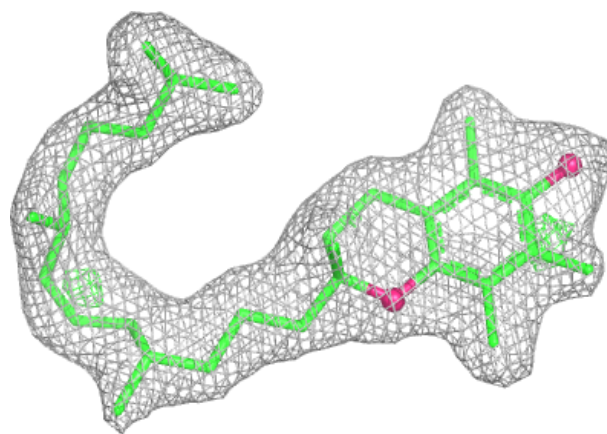


Electron density around PBU B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

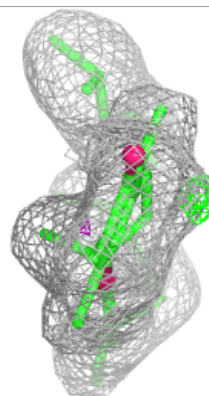
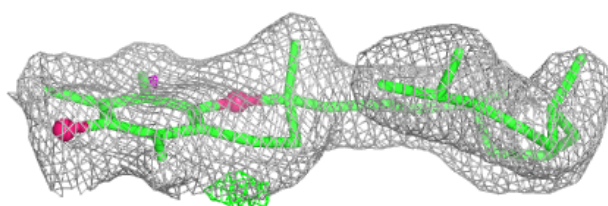
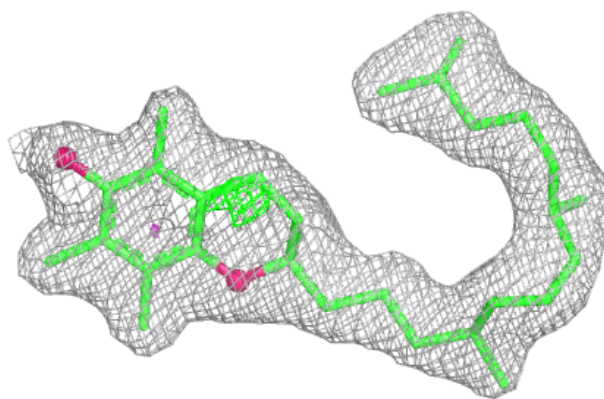
**Electron density around VIV C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

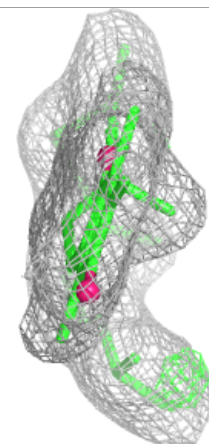
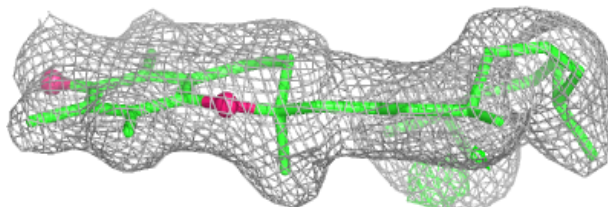
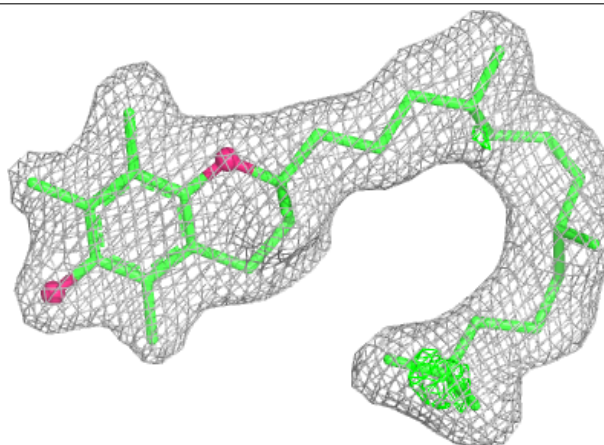


Electron density around VIV B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around VIV A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.